

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau



(43) International Publication Date
18 December 2003 (18.12.2003)

PCT

(10) International Publication Number
WO 03/105058 A2

(51) International Patent Classification⁷: **G06F 19/00**

(21) International Application Number: **PCT/EP03/06049**

(22) International Filing Date: **10 June 2003 (10.06.2003)**

(25) Filing Language: **English**

(26) Publication Language: **English**

(30) Priority Data:
02447115.3 **10 June 2002 (10.06.2002)** **EP**

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(81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Declaration under Rule 4.17:

— of inventorship (Rule 4.17(iv)) for US only

Published:

— without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: **METHOD, COMPUTING ROUTINE, DEVICE FOR PREDICTING PROPERTIES OF MHC/PEPTIDE COMPLEXES, AND DATA AND PEPTIDES PRODUCED THEREFROM**

(57) Abstract: The present invention relates to a method for structure-based prediction of properties of peptides and peptide analogs in complex with major histocompatibility (MHC) class I and class II molecules. The said properties mainly relate to the three-dimensional structure of an MHC/peptide complex and the binding affinity of a peptide for an MHC receptor. The invention further relates to a computer program and a device therefor. The invention further relates to data produced by a method of the invention. The invention further relates to peptides and peptide analogs predicted to bind to target-MHC molecules. The present invention thus relates to the field of immunology, with possible applications in manufacture of vaccines, de-immunization of proteins, and manufacture of therapeutic agents, especially immunotherapeutic agents.

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